Plot scores of training and validation together

This example shows how to plot the scores of principal component 1 and principal component 2 with training and unknown validation data together.

Copyright 2022-2023 Battelle Memorial Institute

Supporting Information

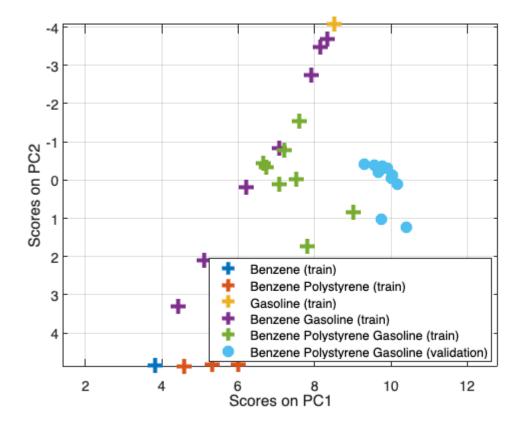
A Practical Guide to Chemometric Analysis of Optical Spectroscopic Data

Hope E. Lackey, ^{1,2} Rachel L. Sell, ¹ Gilbert L. Nelson, ^{3*} Thomas A. Bryan, ^{4*} Amanda M. Lines, ^{1,2*} Samuel A. Bryan, ^{1,2*}

- ¹ Pacific Northwest National Laboratory, 902 Battelle Boulevard, Richland, WA 99352
- ² Washington State University, Department of Chemistry, Pullman WA 99164
- ³College of Idaho, Department of Chemistry, 2112 Cleveland Blvd, Caldwell, ID 83605
- ⁴ The MathWorks, 3 Apple Hill Drive, Natick, MA 01760-2098
- *Email: sam.bryan@pnnl.gov Phone 1 509 375 5648; orcid.org/0000-0002-8826-0880
- *Email: tbryan@mathworks.com Phone 1 508 647 7669
- *Email: amanda.lines@pnnl.gov Phone: 1 509 375 5689
- *Email: gnelson@collegeofidaho.edu Phone: 1 208 459 5241

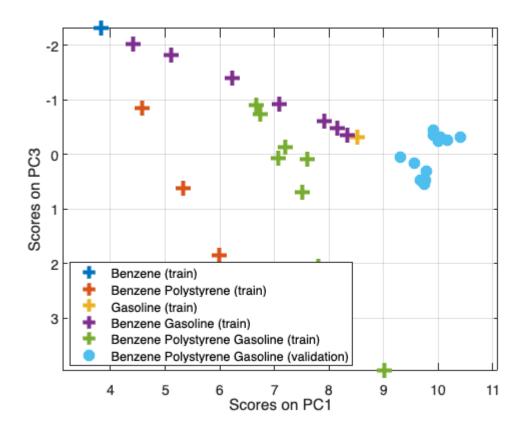
Load and Plot the Data

```
clearvars
load pnnl_napalm_data
first_pca = 1;
second_pca = 2;
displayConcentrations = false;
pnnl_plot_scores_train_vs_unknown(A_train, C_train, A_unknown,
C_validation, first_pca, second_pca, ConstituentNames,
displayConcentrations)
```



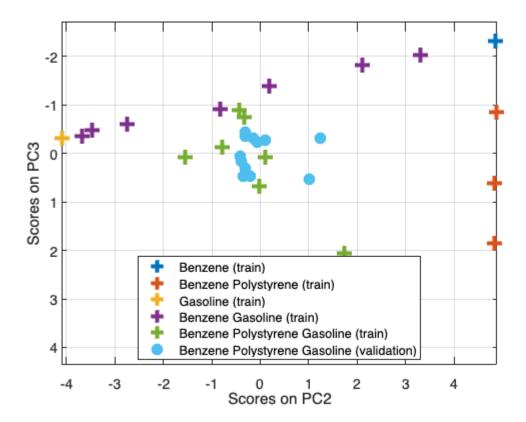
Plot the scores of principal component 1 and principal component 3 with training and unknown validation data together.

```
pnnl_plot_scores_train_vs_unknown(A_train, C_train, A_unknown,
C_validation, 1, 3, ConstituentNames, false)
```



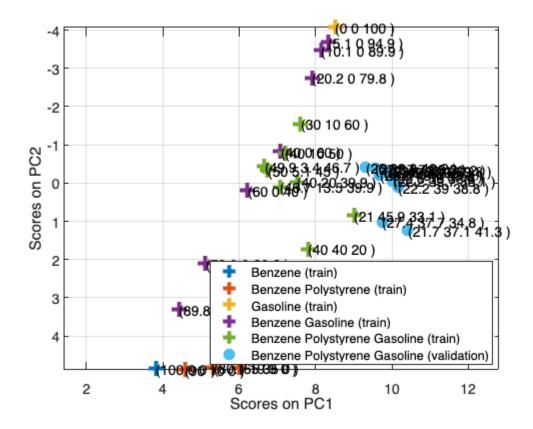
Plot the scores of principal component 2 and principal component 3 with training and unknown validation data together.

```
pnnl_plot_scores_train_vs_unknown(A_train, C_train, A_unknown,
C_validation, 2, 3, ConstituentNames, false)
```



If you set displayConcentrations to true, then the percentages of the concentrations will display on the plot.

```
first_pca = 1;
second_pca = 2;
displayConcentrations = true;
pnnl_plot_scores_train_vs_unknown(A_train, C_train, A_unknown,
C_validation, first_pca, second_pca, ConstituentNames,
displayConcentrations)
```



Disclaimer

This material was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the United States Department of Energy, nor Battelle, nor any of their employees, nor any jurisdiction or organization that has cooperated in the development of these materials, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness or any information, apparatus, product, software, or process disclosed, or represents that its use would not infringe privately owned rights.

Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

operated by

BATTELLE

for the

UNITED STATES DEPARTMENT OF ENERGY

under Contract DE-AC05-76RL01830